

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 13 AUG 2006 HIGHEST RN 901009-82-3
DICTIONARY FILE UPDATES: 13 AUG 2006 HIGHEST RN 901009-82-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

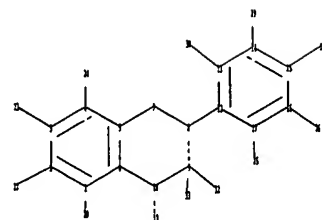
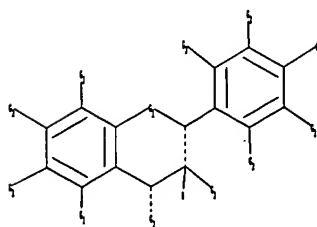
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10762976.str



```

chain nodes :
19 20 22 23 24 25 26 27 29 30 32 33
ring nodes :
1 2 3 4 5 6 7 8 9 10 12 13 14 15 16 17
chain bonds :
1-20 2-22 3-23 4-24 8-12 9-32 9-33 10-19 13-30 14-29 15-27 16-26 17-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 12-13 12-17 13-14 14-15
15-16 16-17
exact/norm bonds :
1-20 2-22 3-23 4-24 5-7 6-10 7-8 8-9 8-12 9-10 9-32 9-33 10-19 13-30
14-29 15-27 16-26 17-25
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17

```

G1:C,O

G2:H,O,F

```

Connectivity :
12:1 M minimum RC ring/chain 13:1 M minimum RC ring/chain 14:1 M minimum RC
ring/chain 15:1 M minimum RC ring/chain 16:1 M minimum RC ring/chain 17:1 M
minimum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:CLASS 22:CLASS
23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 29:CLASS 30:CLASS 32:CLASS
33:CLASS

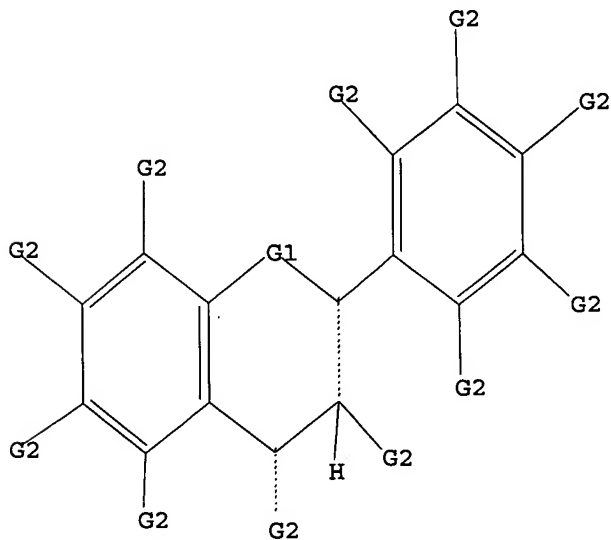
```

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

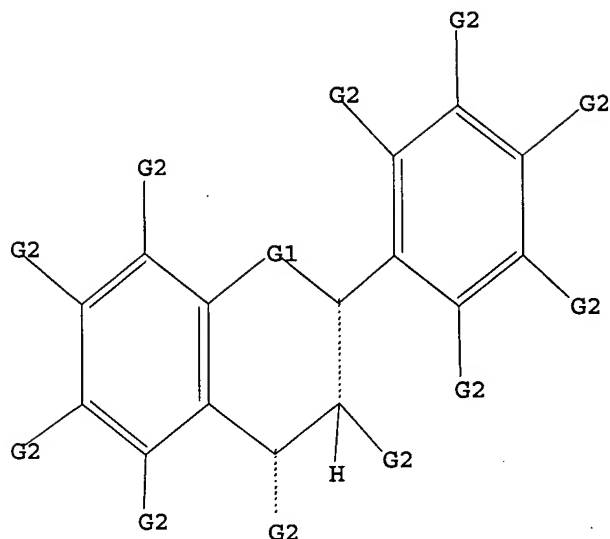


G1 C,O

G2 H,O,F

Structure attributes must be viewed using STN Express query preparation.

=> d l1
 L1 HAS NO ANSWERS
 L1 STR



G1 C,O
 G2 H,O,F

Structure attributes must be viewed using STN Express query preparation.

=> s l1
 SAMPLE SEARCH INITIATED 15:34:33 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 40835 TO ITERATE

4.9% PROCESSED 2000 ITERATIONS 50 ANSWERS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

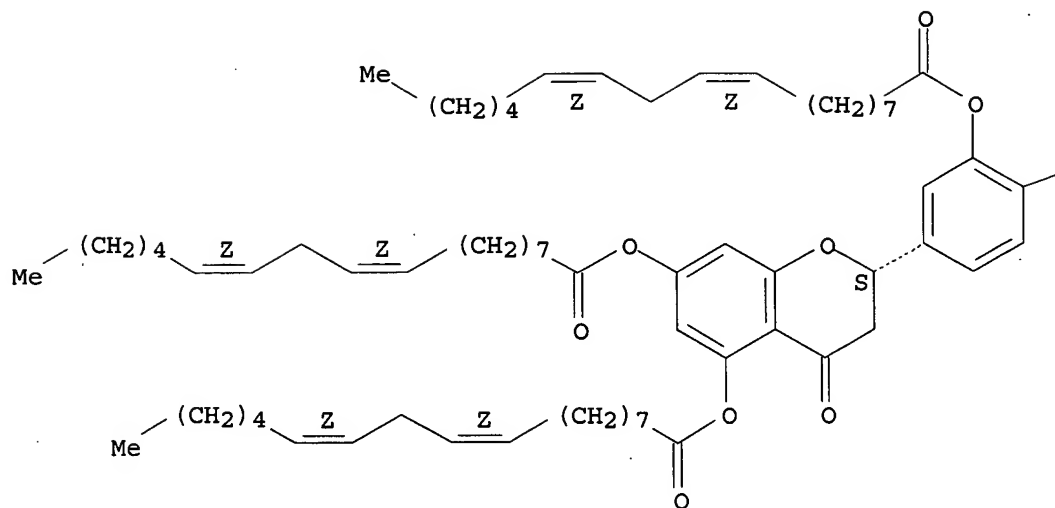
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 804632 TO 828768
 PROJECTED ANSWERS: 19280 TO 23188

L2 50 SEA SSS SAM L1

=> d l2 scan

L2 50 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 9,12-Octadecadienoic acid (9Z,12Z)-, (2S)-3,4-dihydro-2-[4-methoxy-3-
 [[(9Z,12Z)-1-oxo-9,12-octadecadienyl]oxy]phenyl]-4-oxo-2H-1-benzopyran-5,7-
 diyl ester (9CI)
 MF C70 H104 O9

Absolute stereochemistry.
 Double bond geometry as shown.



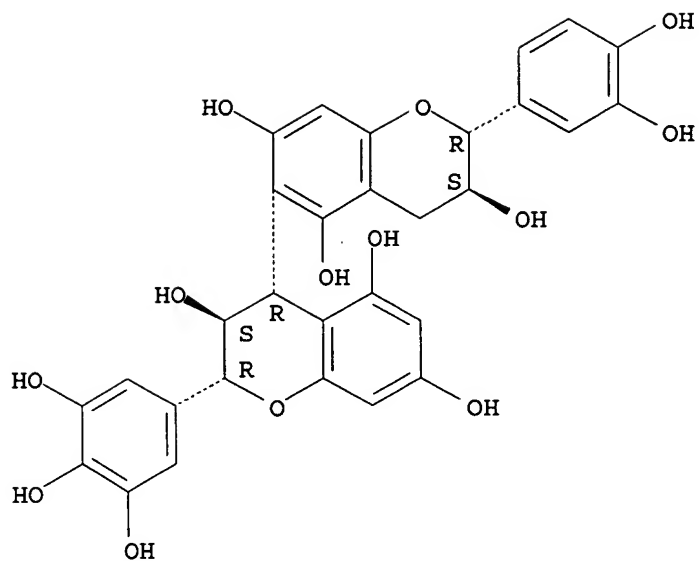
—OMe

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

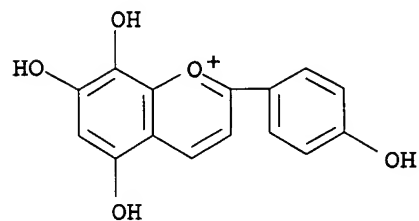
L2 50 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN [4,6'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2'-(3,4-dihydroxyphenyl)-
 3,3',4,4'-tetrahydro-2-(3,4,5-trihydroxyphenyl)-, (2R,2'R,3S,3'S,4R)-
 (9CI)
 MF C30 H26 O13

Absolute stereochemistry.



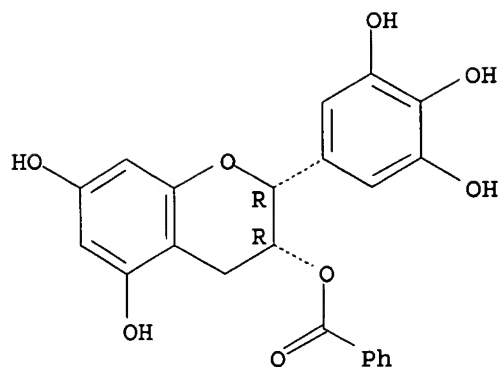
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Flavylum, 4',5,7,8-tetrahydroxy- (8CI)
 MF C15 H11 O5
 CI COM



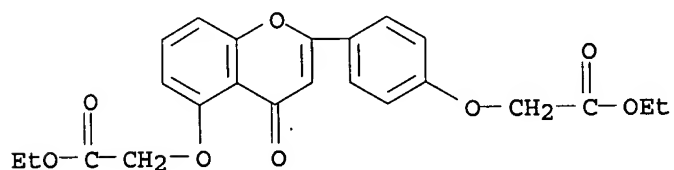
L2 50 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2H-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-,
 3-benzoate, (2R,3R)- (9CI)
 MF C22 H18 O8

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Acetic acid, [[2-[p-(carboxymethoxy)phenyl]-4-oxo-4H-1-benzopyran-5-yl]oxy]-, diethyl ester (7CI)
 MF C23 H22 O8

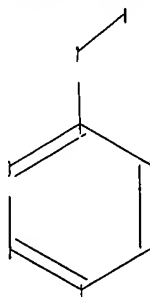
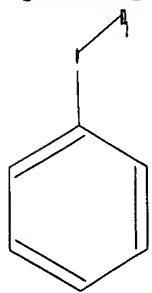


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>

Uploading C:\Program Files\Stnexp\Queries\10762976nitrooxy.str



chain nodes :

7 8

ring nodes :

1 2 3 4 5 6

chain bonds :

4-7 7-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

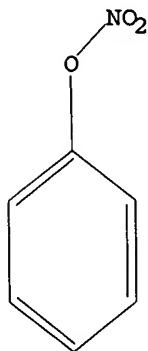
exact/norm bonds :

4-7 7-8
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS

L3 STRUCTURE UPLOADED

=> d l3
L3 HAS NO ANSWERS
L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l3
SAMPLE SEARCH INITIATED 15:35:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 192 TO ITERATE

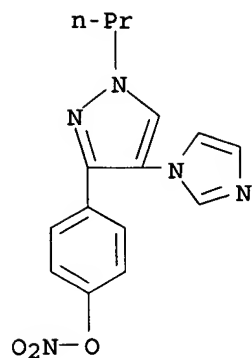
100.0% PROCESSED 192 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3009 TO 4671
PROJECTED ANSWERS: 9 TO 360

L4 9 SEA SSS SAM L3

=> d l4 scan

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Phenol, 4-[4-(1H-imidazol-1-yl)-1-propyl-1H-pyrazol-3-yl]-, nitrate
(ester) (9CI)
MF C15 H15 N5 O3

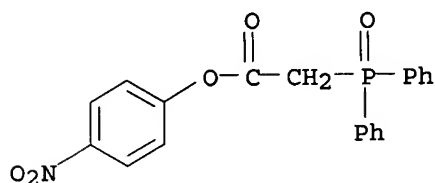


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Acetic acid, (diphenylphosphinyl)-, 4-nitrophenyl ester, compd. with
 phenyl nitrate (1:1) (9CI)
 MF C20 H16 N O5 P . C6 H5 N O3

CM 1



CM 2

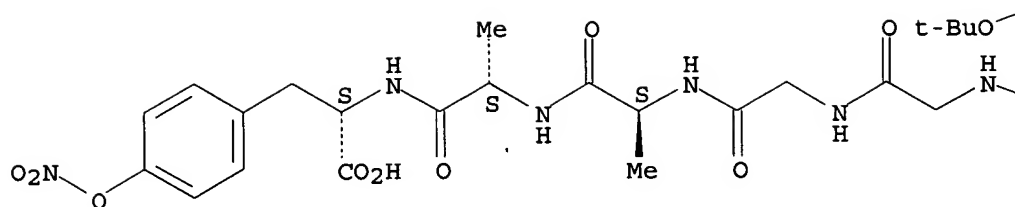
Ph-O-NO₂

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN L-Tyrosine, 3-[2,2'-bibenzoxazol]-5-yl-N-[(1,1-dimethylethoxy)carbonyl]-L-
 alanylglycylglycyl-L-alanyl-L-alanyl-, nitrate (ester) (9CI)
 SQL 6
 MF C41 H45 N9 O14

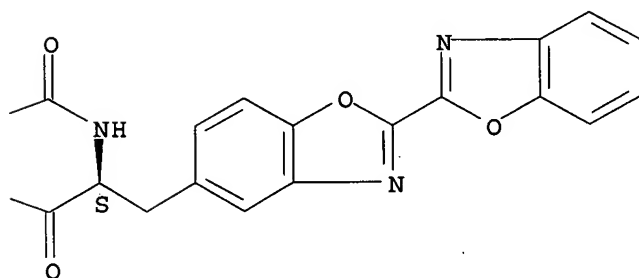
RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

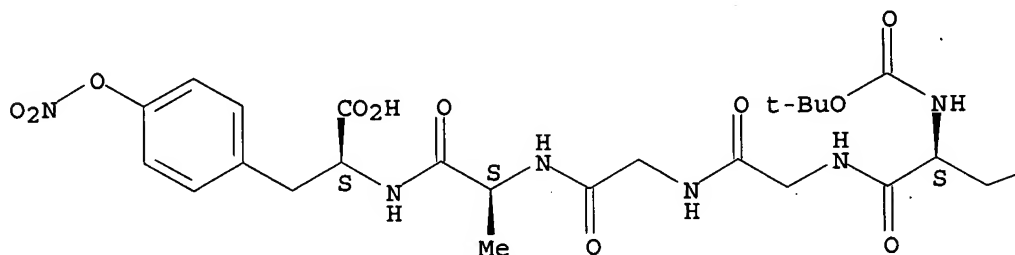


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

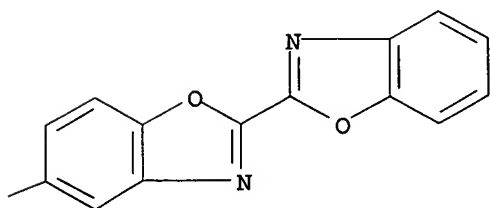
L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN L-Tyrosine, 3-[2,2'-bibenzoxazol]-5-yl-N-[(1,1-dimethylethoxy)carbonyl]-L-alanylglycylglycyl-L-alanyl-, nitrate (ester) (9CI)
 SQL 5
 MF C38 H40 N8 O13

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s l4 and l2

L5 0 L4 AND L2

=> s l4 sss full

FULL SEARCH INITIATED 15:36:10 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 3876 TO ITERATE

100.0% PROCESSED 3876 ITERATIONS

130 ANSWERS

SEARCH TIME: 00.00.01

L6 130 SEA SSS FUL L3

=> s l6 and l2

L7 0 L6 AND L2

=> s l2 sss full

FULL SEARCH INITIATED 15:36:23 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 819203 TO ITERATE

100.0% PROCESSED 819203 ITERATIONS

21448 ANSWERS

SEARCH TIME: 00.00.07

L8 21448 SEA SSS FUL L1

=> s l6 and l8

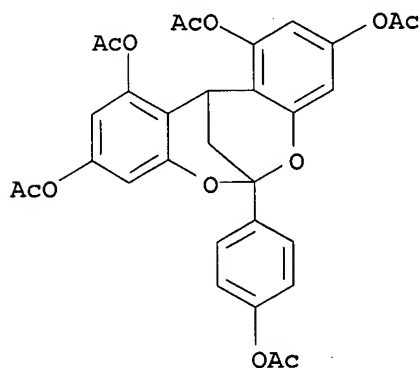
L9 0 L6 AND L8

=> d l8 scan

L8 21448 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C31 H26 O12



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

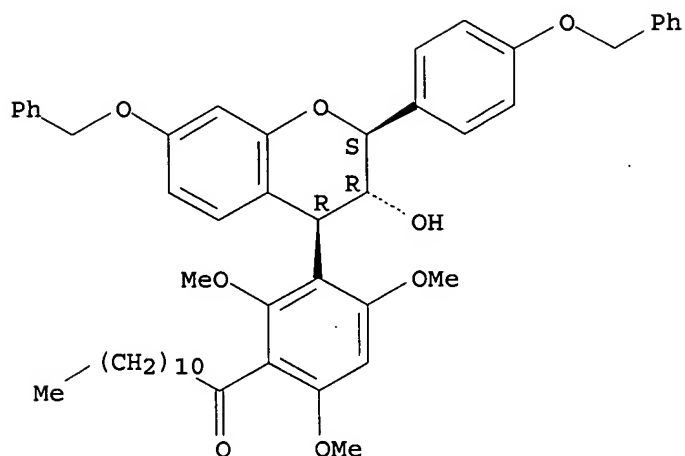
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L8 21448 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1-Dodecanone, 1-[3-[(2S,3R,4R)-3,4-dihydro-3-hydroxy-7-(phenylmethoxy)-2-[4-(phenylmethoxy)phenyl]-2H-1-benzopyran-4-yl]-2,4,6-trimethoxyphenyl]-

(9CI)
MF C50 H58 O8

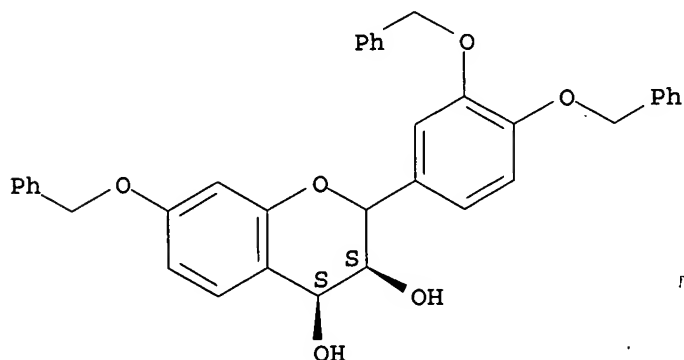
Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

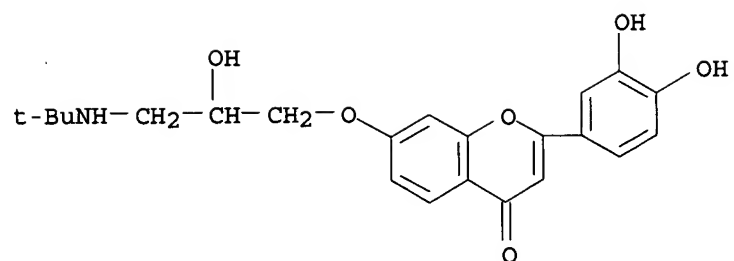
L8 21448 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 3,4-Flavandiol, 3',4',7-tris(benzyloxy)-, cis- (6CI)
MF C36 H32 O6

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 21448 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-7-[3-[(1,1-
dimethylethyl)amino]-2-hydroxypropoxy]- (9CI)
MF C22 H25 N O6



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

FULL ESTIMATED COST

335.64

335.85

STN INTERNATIONAL LOGOFF AT 15:37:17 ON 14 AUG 2006